

**Online Supporting Information S1.** The benchmark dataset contains 8,157 enzyme-drug pair samples, of which 2,719 are interactive and 5,438 non-interactive. All the detailed information for the codes listed here can be found in KEGG database at <http://www.kegg.jp/kegg/>.

<b>Pair attribute</b>	<b>Enzyme code in KEGG</b>	<b>Drug code in KEGG</b>
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Non-interactive	hsa:1178	D00394
Non-interactive	hsa:1178	D01256
Non-interactive	hsa:1200	D00127
Non-interactive	hsa:1200	D00285
Non-interactive	hsa:1200	D00463
Non-interactive	hsa:1200	D01367
Non-interactive	hsa:1200	D02368
Non-interactive	hsa:1200	D04025
Non-interactive	hsa:1215	D00188
Non-interactive	hsa:1215	D00455
Non-interactive	hsa:1215	D00538
Non-interactive	hsa:1215	D01332
Non-interactive	hsa:1215	D02110
Non-interactive	hsa:124	D00283
Non-interactive	hsa:124	D00596
Non-interactive	hsa:124	D00885
Non-interactive	hsa:124	D01240
Non-interactive	hsa:124	D02441
Non-interactive	hsa:125	D00294
Non-interactive	hsa:125	D00455
Non-interactive	hsa:125	D00537
Non-interactive	hsa:1267	D00218
Non-interactive	hsa:1267	D00892
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Non-interactive	hsa:126	D00142

Non-interactive	hsa:126	D00885
Non-interactive	hsa:126	D01332
Non-interactive	hsa:126	D02168
Non-interactive	hsa:126	D03828
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Non-interactive	hsa:128	D03728
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Non-interactive	hsa:130399	D01256
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Non-interactive	hsa:132160	D00070
Non-interactive	hsa:132160	D00315
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Non-interactive	hsa:132	D00107
Non-interactive	hsa:132	D00414
Non-interactive	hsa:132	D00887
Non-interactive	hsa:132	D01275
Non-interactive	hsa:132	D03741
Non-interactive	hsa:133121	D00125
Non-interactive	hsa:134510	D00423
Non-interactive	hsa:134510	D00753
Non-interactive	hsa:134510	D03805
Non-interactive	hsa:1360	D00203
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Non-interactive	hsa:1374	D01211
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Non-interactive	hsa:1376	D01441
Non-interactive	hsa:1376	D02756
Non-interactive	hsa:1376	D03712
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Non-interactive	hsa:1384	D03736
Non-interactive	hsa:1384	D03798
Non-interactive	hsa:13	D00805
Non-interactive	hsa:13	D01718
Non-interactive	hsa:13	D01765
Non-interactive	hsa:13	D02214
Non-interactive	hsa:13	D02368
Non-interactive	hsa:13	D03350
Non-interactive	hsa:142679	D00094
Non-interactive	hsa:142679	D00622
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Non-interactive	hsa:142679	D01240
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Non-interactive	hsa:1431	D02194
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Non-interactive	hsa:1432	D00359
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Non-interactive	hsa:1432	D00414



Non-interactive	hsa:1432	D00781
Non-interactive	hsa:1436	D00963
Non-interactive	hsa:1436	D02655
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Non-interactive	hsa:1445	D00216
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Non-interactive	hsa:1445	D01256
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Non-interactive	hsa:1445	D02375
Non-interactive	hsa:1445	D03767
Non-interactive	hsa:1445	D03806
Non-interactive	hsa:150290	D00655
Non-interactive	hsa:1504	D00328
Non-interactive	hsa:1504	D00448
Non-interactive	hsa:1504	D00533
Non-interactive	hsa:1504	D01866
Non-interactive	hsa:1504	D03689
Non-interactive	hsa:151531	D00218
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Non-interactive	hsa:151531	D03710
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Non-interactive	hsa:1537	D00650
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Non-interactive	hsa:1562	D00070
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Non-interactive	hsa:1562	D00813
Non-interactive	hsa:1562	D00965
Non-interactive	hsa:1562	D01211

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Non-interactive	hsa:1565	D01918
Non-interactive	hsa:1571	D00387
Non-interactive	hsa:1571	D00753
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Non-interactive	hsa:1571	D02042
Non-interactive	hsa:1572	D00892
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Non-interactive	hsa:1572	D01767
Non-interactive	hsa:1572	D01844
Non-interactive	hsa:1572	D03735
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Non-interactive	hsa:1573	D01918
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Non-interactive	hsa:1849	D00218
Non-interactive	hsa:1849	D02328
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Non-interactive	hsa:1850	D00752
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Non-interactive	hsa:1852	D01765
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Non-interactive	hsa:189	D01578
Non-interactive	hsa:189	D02229
Non-interactive	hsa:189	D02258
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Non-interactive	hsa:18	D02418
Non-interactive	hsa:191	D00142
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Non-interactive	hsa:2050	D00142
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Non-interactive	hsa:2050	D03735
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Non-interactive	hsa:2147	D03350
Non-interactive	hsa:2147	D03758
Non-interactive	hsa:2147	D03767
Non-interactive	hsa:2155	D00387
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Non-interactive	hsa:223	D03736
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Non-interactive	hsa:23239	D01973
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Non-interactive	hsa:3990	D00398
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Non-interactive	hsa:3990	D03440
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Non-interactive	hsa:3991	D00328
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Non-interactive	hsa:4023	D02166
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Non-interactive	hsa:4128	D01133
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Non-interactive	hsa:4128	D01367
Non-interactive	hsa:4128	D02168
Non-interactive	hsa:4129	D03828
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Non-interactive	hsa:4282	D02560
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Non-interactive	hsa:4311	D00216
Non-interactive	hsa:4311	D00652
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Non-interactive	hsa:43	D03736
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Non-interactive	hsa:444	D00651
Non-interactive	hsa:444	D00658
Non-interactive	hsa:444	D00805
Non-interactive	hsa:444	D00892
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Non-interactive	hsa:51727	D03440
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Non-interactive	hsa:6768	D00651
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Non-interactive	hsa:51172	D00434
Non-interactive	hsa:231	D00398
Non-interactive	hsa:5156	D01966
Non-interactive	hsa:4593	D01211
Non-interactive	hsa:7046	D00703
Non-interactive	hsa:6652	D00007
Non-interactive	hsa:5479	D00691
Non-interactive	hsa:56922	D01840
Non-interactive	hsa:1728	D00998
Non-interactive	hsa:5332	D00521
Non-interactive	hsa:23475	D02729
Non-interactive	hsa:5141	D04029
Non-interactive	hsa:660	D00387
Non-interactive	hsa:9955	D00709
Non-interactive	hsa:1633	D01966
Non-interactive	hsa:5406	D03034
Non-interactive	hsa:5050	D00094



Non-interactive	hsa:10935	D02315
Non-interactive	hsa:2180	D00333
Non-interactive	hsa:7299	D02451
Non-interactive	hsa:5335	D00691
Non-interactive	hsa:196883	D00691
Non-interactive	hsa:1384	D01667
Non-interactive	hsa:10924	D00410
Non-interactive	hsa:10941	D01228
Non-interactive	hsa:56922	D01665
Non-interactive	hsa:63904	D03712
Non-interactive	hsa:657	D00475
Non-interactive	hsa:7525	D00423
Non-interactive	hsa:260293	D00459
Non-interactive	hsa:100	D01888
Non-interactive	hsa:5494	D00118
Non-interactive	hsa:91	D00300
Non-interactive	hsa:3906	D00703
Non-interactive	hsa:51302	D00726
Non-interactive	hsa:5095	D01275
Non-interactive	hsa:81579	D00892
Non-interactive	hsa:7054	D02835
Non-interactive	hsa:767	D02355
Non-interactive	hsa:5651	D01977
Non-interactive	hsa:9088	D02564
Non-interactive	hsa:5837	D00882
Non-interactive	hsa:759	D01432
Non-interactive	hsa:4548	D03670
Non-interactive	hsa:8555	D02451
Non-interactive	hsa:3033	D00904
Non-interactive	hsa:3791	D00391
Non-interactive	hsa:7364	D00340
Non-interactive	hsa:760	D03689
Non-interactive	hsa:1969	D00387
Non-interactive	hsa:2597	D00274
Non-interactive	hsa:131	D00103
Non-interactive	hsa:1549	D02258
Non-interactive	hsa:3028	D01276
Non-interactive	hsa:6652	D00709
Non-interactive	hsa:223	D00070
Non-interactive	hsa:695	D00449
Non-interactive	hsa:3615	D00328
Non-interactive	hsa:7371	D00653

Non-interactive	hsa:8836	D00452
Non-interactive	hsa:5595	D03767
Non-interactive	hsa:6898	D03826
Non-interactive	hsa:3712	D00434
Non-interactive	hsa:5159	D00826
Non-interactive	hsa:109	D01425
Non-interactive	hsa:7010	D02562
Non-interactive	hsa:5319	D00139
Non-interactive	hsa:55811	D01071
Non-interactive	hsa:5501	D03743
Non-interactive	hsa:51302	D02166
Non-interactive	hsa:5137	D03440
Non-interactive	hsa:3988	D01441
Non-interactive	hsa:1384	D01198
Non-interactive	hsa:5533	D03828
Non-interactive	hsa:91039	D00391
Non-interactive	hsa:5523	D03781
Non-interactive	hsa:2638	D00653
Non-interactive	hsa:4953	D01765
Non-interactive	hsa:217	D01718
Non-interactive	hsa:2264	D03788
Non-interactive	hsa:5122	D00656
Non-interactive	hsa:54577	D00380
Non-interactive	hsa:7298	D01918
Non-interactive	hsa:3612	D00566
Non-interactive	hsa:55312	D00452
Non-interactive	hsa:4837	D01064
Non-interactive	hsa:2534	D00902
Non-interactive	hsa:1537	D02229
Non-interactive	hsa:109	D03751
Non-interactive	hsa:5860	D00018
Non-interactive	hsa:5095	D02560
Non-interactive	hsa:5743	D01715
Non-interactive	hsa:5599	D00562
Non-interactive	hsa:93	D00752
Non-interactive	hsa:5330	D00651
Non-interactive	hsa:10825	D03722
Non-interactive	hsa:4759	D00960
Non-interactive	hsa:4837	D00654
Non-interactive	hsa:1585	D00650
Non-interactive	hsa:10747	D01709
Non-interactive	hsa:657	D03218

Non-interactive	hsa:6652	D00283
Non-interactive	hsa:5406	D01367
Non-interactive	hsa:5516	D02323
Non-interactive	hsa:57176	D03433
Non-interactive	hsa:11330	D00298
Non-interactive	hsa:5340	D00196
Non-interactive	hsa:5602	D00279
Non-interactive	hsa:1544	D02729
Non-interactive	hsa:4482	D00533
Non-interactive	hsa:54600	D00650
Non-interactive	hsa:23475	D01984
Non-interactive	hsa:7367	D03722
Non-interactive	hsa:5532	D00829
Non-interactive	hsa:5050	D01907
Non-interactive	hsa:5033	D03743
Non-interactive	hsa:7366	D03601
Non-interactive	hsa:3295	D00889

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